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Massively Parallel Reactive and Quantum Molecular Dynamics Simulations

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In this talk I will discuss two simulations: Cavitation bubbles readily occur in fluids subjected to rapid changes in pressure. We use billion-atom reactive molecular dynamics simulations on a 163,840-processor BlueGene/P supercomputer to investigate chemical and mechanical damages caused by shock-induced collapse of nanobubbles in water near silica surface. Collapse of an empty nanobubble generates high-speed nanojet, resulting in the formation of a pit on the surface. The gas-filled bubbles undergo partial collapse and consequently the damage on the silica surface is mitigated. Quantum molecular dynamics (QMD) simulations are performed on 786,432-processor Blue Gene/Q to study on-demand production of hydrogen gas from water using Al nanoclusters. QMD simulations reveal rapid hydrogen production from water by an Al nanocluster. We find a low activation-barrier mechanism, in which a pair of Lewis acid and base sites on the Al_n surface preferentially catalyzes hydrogen production. I will also discuss on-demand production of hydrogen gas from water using and LiAl alloy particles. Research reported in this lecture was carried in collaboration with Rajiv Kalia, Aiichiro Nakano and Ken-ichi Nomura from the University of Southern California, and Fuyuki Shimojo and Kohei Shimamura from Kumamoto University, Japan.